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## Disclaimer

# Coherent Diffractive Imaging Using Curved-Beam Illumination

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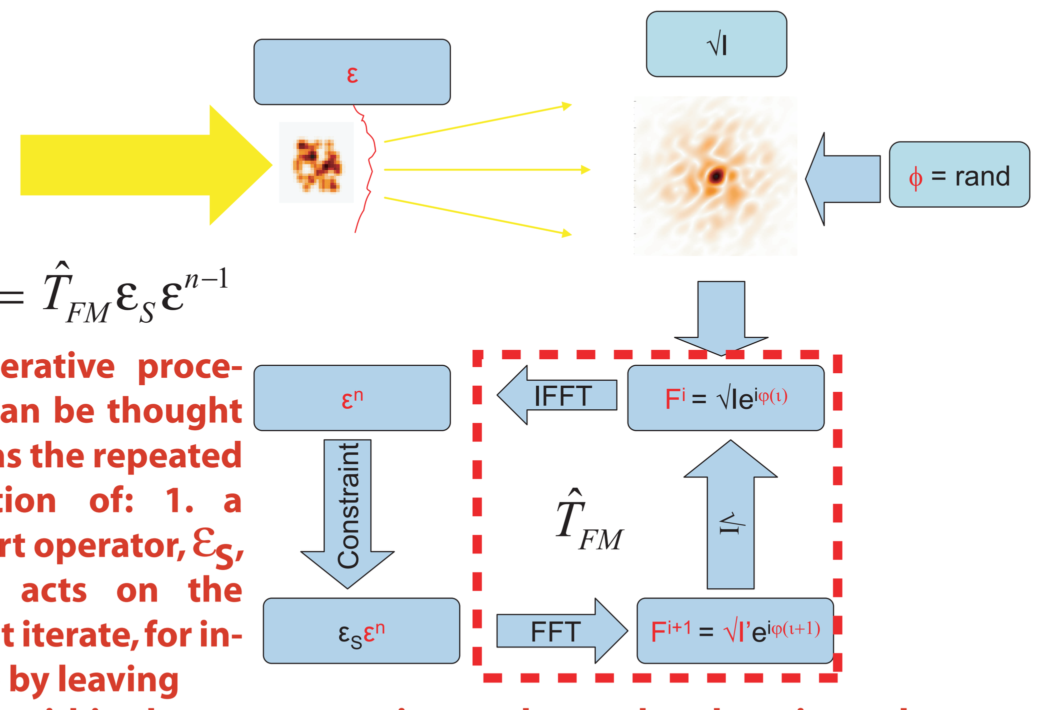
## Introduction

The potential of coherent diffractive imaging has in recent years become well recognised. In this technique an essentially parallel beam of coherent x-rays illuminates a support region containing an unknown sample. Outside that region the wavefield is known - typically the sample is isolated so that outside the support there is no scattering. When the diffraction pattern is measured with sufficient signal to noise ratio an iterative technique can be used to solve for the transmission funcion of the sample. The technique offers extremely high resolution reconstructions of a sample.



$$\varepsilon^n = \hat{T}_{FM}\varepsilon_S\varepsilon^{n-1}$$

The iterative procedure can be thought of [1] as the repeated operation of: 1. a support operator, $\varepsilon_S$, which acts on the current iterate, for instance by leaving values within the support region unchanged and setting values outside to zero; and 2. a Fourier modulus operator, $\hat{T}_{FM}$, which fourier transforms the iterate as updated by the support information, sets the measured amplitude and inverse Fourier transfoms the result back to obtain the next iterate.

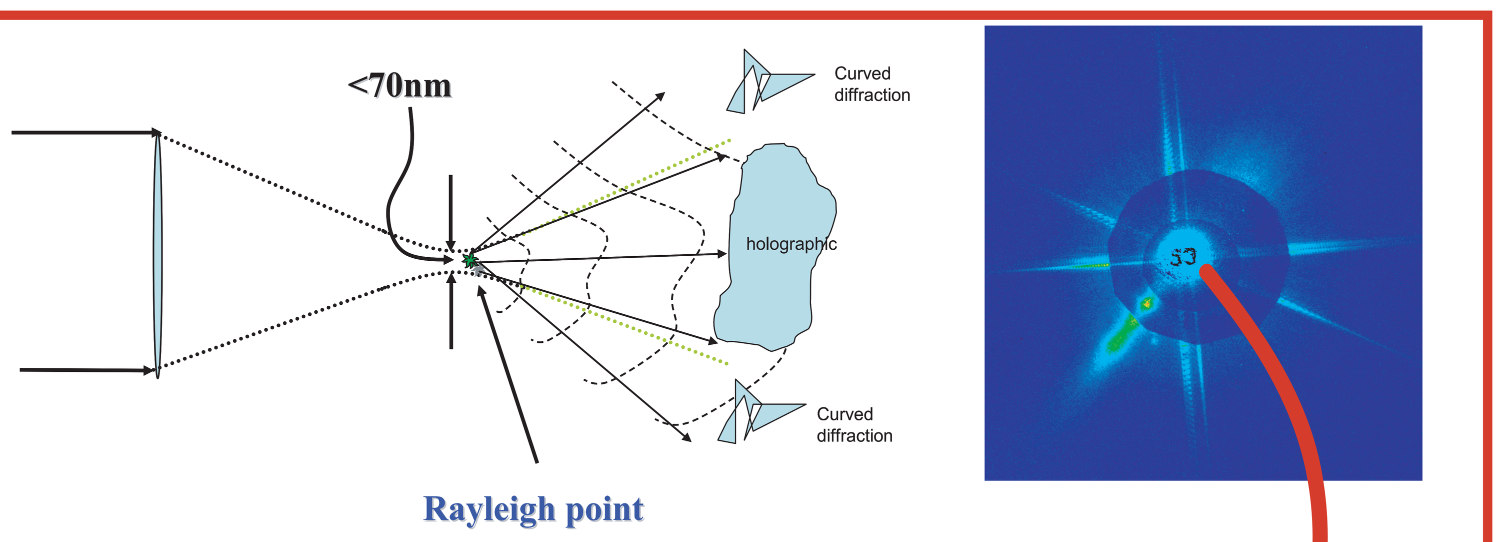
## Curved Beam Illumination

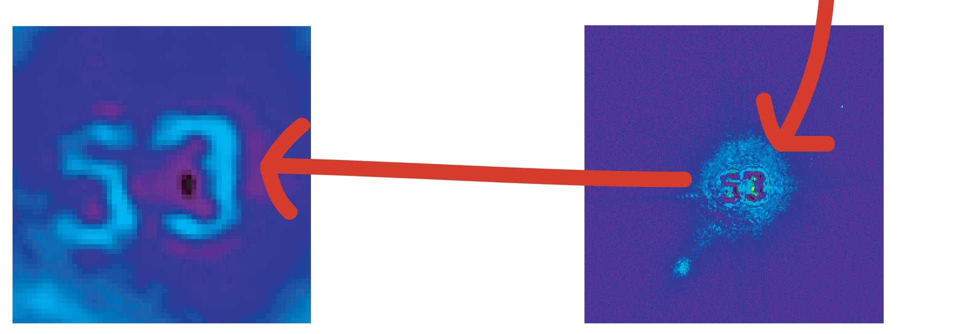
Here we consider the effect of illuminating the sample with a beam that has significant curvature over the width of the sample. This can be achieved by using a focusing optic such as a zone plate and positioning the sample a short distance from the focal point. We describe the following results [1,2,3]:

- *Low Frequency Starting Estimate*
- *No Support Convergence*
- *Unique Solutions*
- *How Much Curvature is Required*
- *Faster Convergence*
- *Large and Periodic Object Convergence*
- *Effect of Imperfect Knowledge of Beam Curvature*

## Low Frequency Starting Estimate

The diffraction pattern resulting from curved beam illumination is different to that arising from plane wave illumination. In the far field there will be a region corresponding to the numerical aperture of the focusing optic. Within this region the diffraction from the sample will interfere with the defocused beam from the optic producing an in-line hologram of the sample. This can be inverted to produce a low-resolution (limited to the resolution of the optic) estimate of the sample. This estimate can be used to provide a compact support region

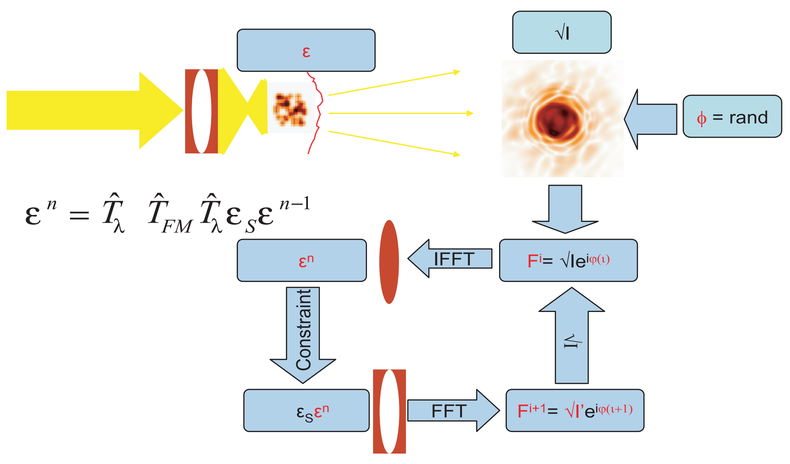


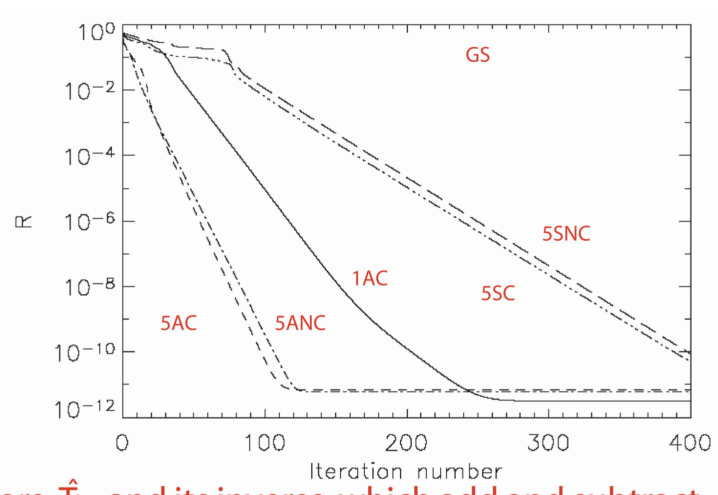
**Maximal beam curvature is obtained at the Raleigh point. The resulting diffraction pattern is holographic within the expanding beam diameter and is comprised of scattered signal from the sample outside this region. Data from a microfabricated gold numeral "50" which has been contrast enhanced in three regions is shown. From the central holographic region a reconstruction of the sample is shown. Part of the sample has been obscured by the zone plate beam stop.**

## Faster Convergence

The effect of encoding a reference phase onto different spatial locations on the sample appears to provide an additional positive feedback mechanism in the iterative procedure and produces faster convergence rates when obtaining a solution [2]. Additional schemes which also speed up convergence include the use of multiple diffraction data sets under conditions of different amounts of curvature in the illuminating illumination and the use of asymmetric curvature, such as pairs of orthogonally oriented cylindrical curvatures. Under these schemes additional operators are required in the iterative scheme which add and subtract the effect of the various beam curvatures.



$$\varepsilon^n = \hat{T}_\lambda\hat{T}_{FM}\hat{T}_\lambda\varepsilon_S\varepsilon^{n-1}$$



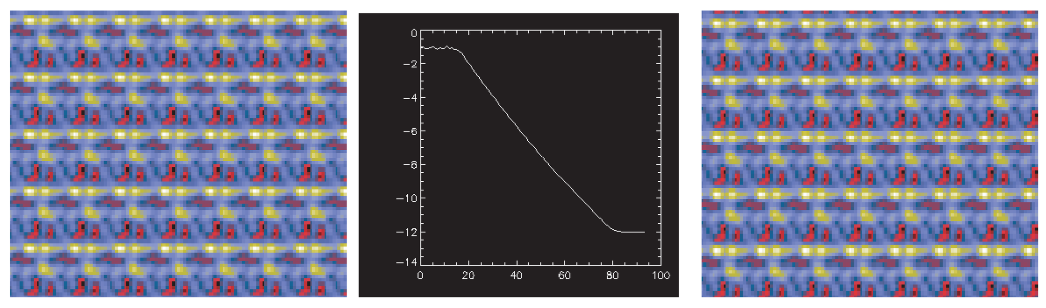

Curved beam illumination requires that additional operators, $\hat{T}_\lambda$, and its inverse, which add and subtract the effects of the beam curvature, be included. When multiple or asymmetric curvatures are used the operator corresponding to the appropriate curvature is used. In numerical tests the use of multiple (curves labelled with "5" for 5 different curvatures) and asymmetric curvatures (curves labelled with "A" for asymmetric) greatly enhances convergence time. The traditional plane wave approach (curve labelled "GS") has not deviated significantly from the top of the graph in the number of iterations shown.

## No Support Convergence

Under conditions when multiple curvature datasets are used the beam curvature operators are a sufficient constraint and the finite support region operator can be discarded. When this is done convergence is only marginally slower (curves labelled with "NC" on the graph to the left) than when the finite support operator is retained (curves labelled with "C") [2].

## Large and Periodic Object Convergence

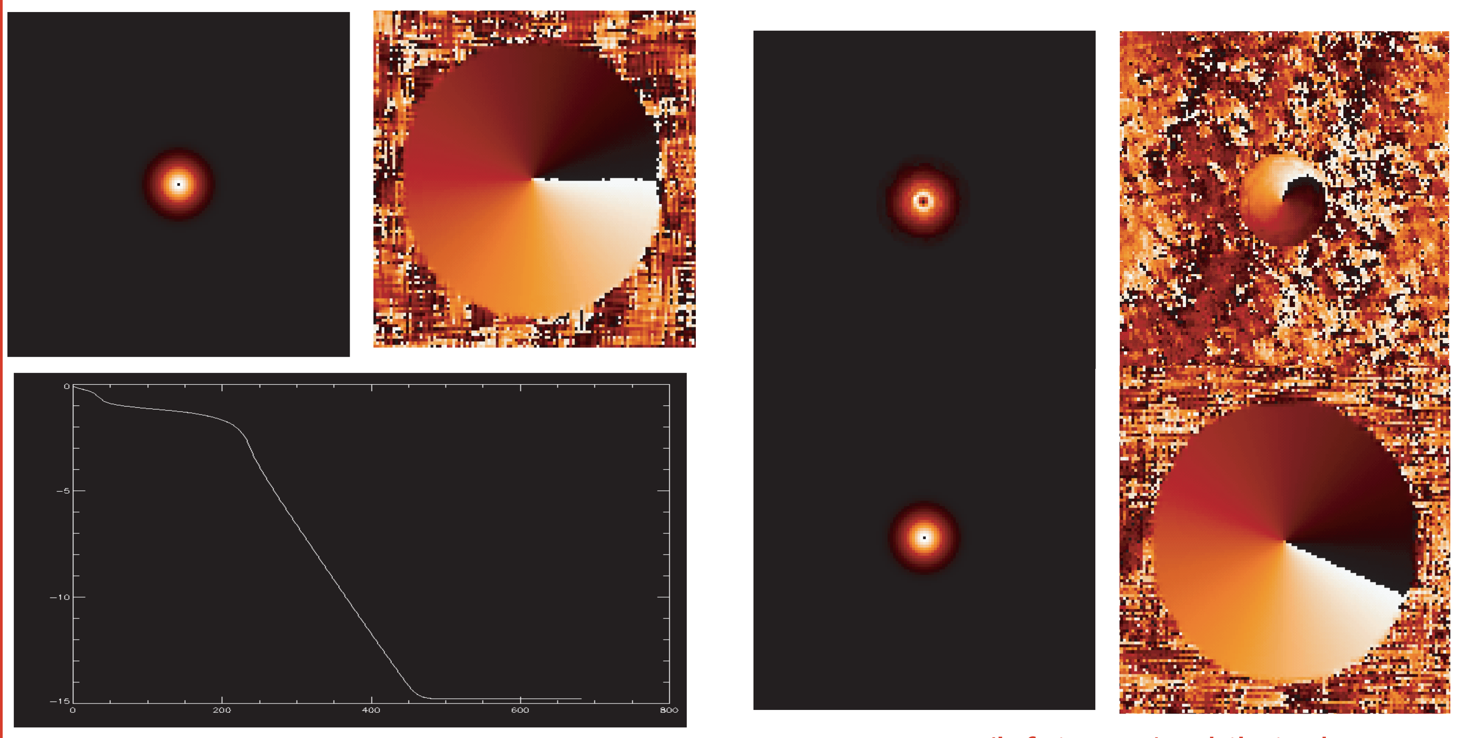
It follows that the sample need no longer be finite in size. Effectively the beam decay to zero apertures the sample in a way characteristic of a finite sample. This means that large, and more importantly, periodic objects may be reconstructed. For periodic objects we have additionally shown that knowledge of the unit cell dimension allows a unique solution [2].



Sample and its reconstruction using multiple asymmetrically curved data sets. The convergence plot shows a typically rapid convergence.

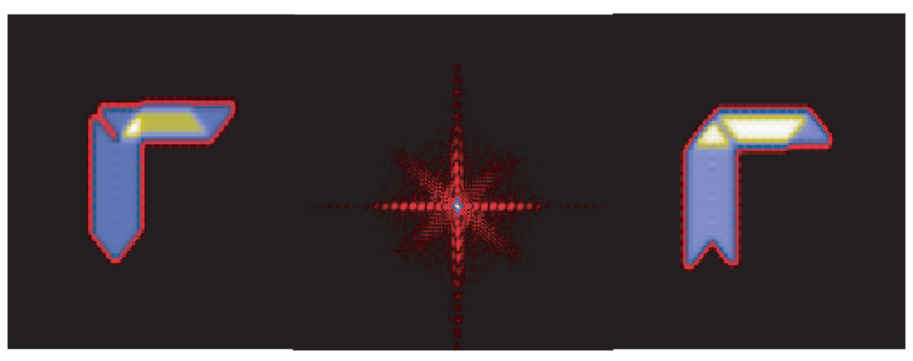
## Unique Solutions

In addition to the special case of periodic samples, we have shown that the use of asymmetric (sometimes called astigmatic) curvature will guarantee a unique solution is obtained [3]. This is true even in cases which are generally pathological for other phase retrieval methods.



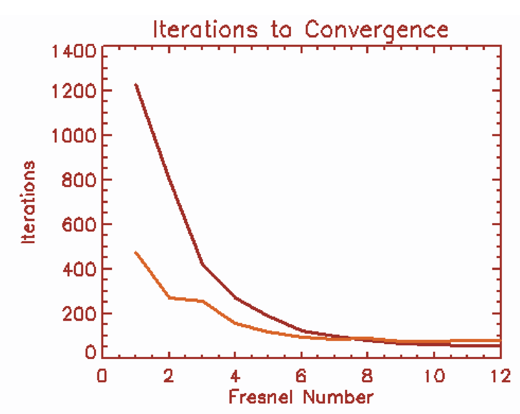
The optical vortex is characterised by a point singularity about which a donut shaped intensity distribution is seen (upper left plot) [4,5,6]. An integer multiple of a $2\pi$ phase ramp circulates about the singularity (next to upper left plot). The symmetry in the intensity is preserved on a reversal of the direction of the phase ramp. Consequently, the plane wave method (shown in the top right pair of plots) and the spherically curved beam method (as well as other phase retrieval methods) cannot reconstruct the sign of the phase helicity [4]. Note the phase ramp is reversed. However, using asymmetric curvature introduces distortions in the measured intensity that relates to the helicity thus introducing information sufficient to retrieve the phase ramp direction (shown in the bottom right pair of plots). The characteristic speed of convergence is also retained as shown in the lower left plot.

An additional pathology arises for so-called homometric objects. In this case a sample can be described as the convolution of a basis with a kernel (left image), while its homometric pair is the convolution of the same basis with the spatially reversed conjugate of the kernel (right image). It is straightforward to show that such objects produce identical diffraction patterns (centre image). Accordingly, when the kernel is not conjugate-spatially symmetric we have a new class of object that is not "trivially" symmetric that cannot be solved by the standard methods of coherent diffractive imaging. Such objects need not be rare - one can envisage micro- or nano-fabricated samples that satisfy this criterion. We have shown that under asymmetrically curved illumination the orthogonal distortions introduce additional information that allow a unique solution to be obtained (our solutions are identical by eye to the images shown) [2].



## How Much Curvature is Required?

While in general increasing curvature will improve convergence rates, we have demonstrated that the increase in convergence rate diminishes with increasing curvature, In any event, large curvatures are practically difficult to obtain. Numerical simulations indicate that beyond a Fresnel number (corresponding to the number of cycles of $2\pi$ in phase curvature across the object) of about 5 there is little practical improvement [1].




Number of iterations to convergence for two samples as a function of Fresnel number.

$$\varepsilon_o^n = \hat{T}_\lambda^{-1}\hat{T}_{FM}\hat{T}_\lambda\varepsilon_S\hat{T}_\lambda^{-1}\hat{T}_{FM}\hat{T}_\lambda\varepsilon_S\varepsilon_o^{n-2}$$

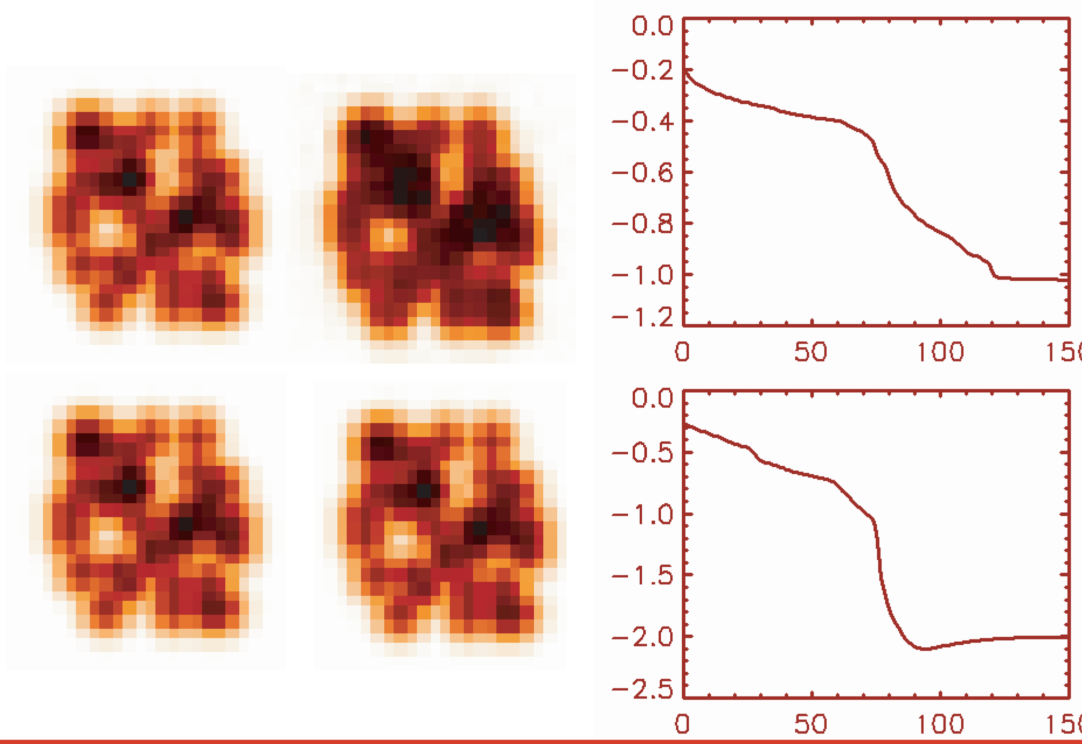
$$\varepsilon_S = \begin{matrix} 1 & \mathbf{r}\in S \\ 0 & \mathbf{r}\notin S \end{matrix}$$

$$\hat{T}_\lambda = A\exp\left(-\mu_r r^2\right)\exp\left(-\mu_i r^2\right)$$

$$\hat{T}_\lambda^{-1} = \frac{1}{A}\exp\left(\mu_r r^2\right)\exp\left(\mu_i r^2\right)$$

## Effect of Imperfect Knowledge of Beam Curvature

If we consider a reconstruction using a single spherical curvature then we can expand the sequence of operators over two cycles as shown. In general the beam curvature operators will commutate with the finite support operator so that apart from the first and last beam curvature operators they cancel. Consequently any errors in the characterisation of the beam will tend to cancel and there should be minimal effect on the reconstruction. We tested this numerically where the error in the beam corresponded to an error in the Fresnel number for the illuminating beam (this could also correspond to an error in knowing the distance from the beam focus to the sample). Acceptable reconstructions are obtained even for relatively large beam errors.



For multiple curvatures introduced by moving the source relative to the focus, there will be a constant difference between successive beam subtraction and beam addition operators. Where there are beam characterisation errors a constant correction factor can be found to obtain the correct difference and the resulting reconstruction should be affected qualitatively in the same way as for the single plane case.

The bottom three images show respectively the sample, its reconstruction and the convergence plot under the condition where there is a 1% error in the characterisation of the Fresnel number of the illuminating beam. The top three images show the same information for the case of a 10% error. Very little discernable difference is observed for the 1% error case. For the 10% error case a good reconstruction is still seen although some differences are now apparent.

## Conclusions

We are currently undertaking a range of experimental investigations in order to confirm our arguments and to investigate the practical difficulties of undertaking coherent diffractive imaging using curved beam illumination.

### References

[1] H. M. Quiney, K. A. Nugent, A. G. Peele "Iterative image reconstruction algorithms using wavefront intensity and phase variation," Optics. Lett., Accepted (2005)
[2] K. A. Nugent, A. G. Peele, H. M. Quiney, "Diffraction with WavefrontCurvature: A Path to Unique Phase Recovery," Acta Cryst. A61, 373 – 381(2005).
[3] K.A.Nugent, A.G.Peele, H.N.Chapman and A.P.Mancuso, "Unique Phase Recovery for Non-Periodic Objects," Phys. Rev. Lett., 91, 203902 (2003)
[4] A. G. Peele, K. A. Nugent, A. P. Mancuso, D. Paterson, I. McNulty, J. P. Hayes, "X-Ray Vortices:Theory and Experiment," J. Opt. Soc. Am. A, 21, 1575-1584 (2004)
[5] A. G. Peele and K. A. Nugent, "X-Ray Vortex Beams: A Theoretical Analysis," Opt. Expr., 11, 2315 (2003)
[6] A. G. Peele, P. J. McMahon, D. Paterson, C. Q. Tran, A. Mancuso, K. A. Nugent, J. P. Hayes, E. Harvey, B. Lai I. McNulty "Observation of an X-ray Vortex", Opt. Lett. 27, 1752-1754 (2002).

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